L Number	Hits	Search Text	DB	Time stamp
1	1328	((544/250) or (544/252) or (544/282) or	USPAT;	2004/03/04 11:53
		(514/259.4) or (514/259.41) or	US-PGPUB;	
		(514/267)).CCLS.	EPO; JPO;	
			DERWENT	

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C:\STNEXP4\QUERIES\10620240.str
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ring nodes :
    1 2 3 4 5
                             9 10 15 16 17 18 19 20
chain bonds :
    10-12 13-17
ring bonds :
    1 - 2 \quad 1 - 6 \quad 2 - 3 \quad 3 - 4 \quad 4 - 5 \quad 5 - 6 \quad 5 - 7 \quad 6 - 10
                                              7-8
                                                    8-9
                                                          9-10 15-16 15-20 16-17 17-18 18-19
    19-20
exact/norm bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 10-12
exact bonds :
    13-17
normalized bonds :
    15-16 15-20 16-17 17-18 18-19 19-20
```

G1:0,N

G2:0,S,N,SO2

chain nodes: 12 13 22

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:CLASS 13:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 22:CLASS 23:CLASS

=>

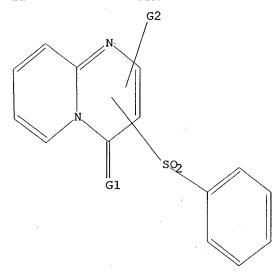
Uploading 10620240.str

STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

STR



G1 O, N

G2 O, S, N, SO2

Structure attributes must be viewed using STN Express query preparation.

=> s 11 sss sam

SAMPLE SEARCH INITIATED 16:17:07 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 45 TO ITERATE

100.0% PROCESSED

45 ITERATIONS

2 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS:

498 TO

PROJECTED ANSWERS:

2 TO

L2

2 SEA SSS SAM L1

=> s l1 sss ful

FULL SEARCH INITIATED 16:17:33 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 934 TO ITERATE

100.0% PROCESSED 934 ITERATIONS

45 ANSWERS

SEARCH TIME: 00.00.01

45 SEA SSS FUL L1

=> s 13

L4

2 L3

=> d 14 1-2 bib,ab,hitstr

L4ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN

ΑN 2004:80350 CAPLUS

Preparation of pyridopyrimidines as 5-HT6 antagonists TT.

Wu, Yong-jin; Hu, Shuanghua; Scola, Paul M.; Huang, Yazhong; Grant-Young, IN Katharine A.

PA

U.S. Pat. Appl. Publ., 19 pp. SO

CODEN: USXXCO

DT Patent

English LΑ

FAN.

FAN.CNT	_				
PA	TENT NO.	KIND	DATE	APPLICATION NO.	DATE
				<b></b>	
PI US	2004019064	A1	20040129	US 2003-620240	20030715
PRAI US	2002-398929P	P	20020726		

The title compds. [I; R1 = (un)substituted naphthyl, Ph; R2 = 5-methylpyridin-2-yl, alkyl, hydroxyalkyl; R3 = H, halo, alkyl, benzyloxy; R4 = H, alkyl; R3 and R4 together, optionally form a 5-6 membered aryl having 0-2 heteroatoms; R5 = H, halo, alkyl, CH2Ph, COR8; X = NR6, O, SOm; Y = NR7, O; m = 0-2; R6 = H, alkyl; R7 = H, alkyl, CO(alkyl); R8 = alkoxy, (un) substituted NH2, OH] which have a binding affinity for the human 5-HT6 receptor and, therefore, are useful in treating disorders responsive to antagonism of the 5-HT6 receptor such as psychosis, schizophrenia, manic depression, depression, neurol. disorder, memory disorder, Parkinson's disease, amyotrophic lateral sclerosis, Alzheimer's disease and Huntington's chorea, were prepd. Prepn. of 35 compds. I is described. The compds. I were tested for binding at the 5-HT6 receptor. E.g., I [R1 = 4-ClC6H4; R2 = Me; R3-R5 = H; X = S; Y = NH] showed IC50 of <20 nM against 5-Ht6 binding. Pharmaceutical compn. comprising the compd. I is claimed.

## 614732-18-2P IT

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (prepn. of pyridopyrimidines as 5-HT6 antagonists)

RN 614732-18-2 CAPLUS

CN 4H-Pyrido[1,2-a]pyrimidin-4-imine, 2-(methylthio)-3-(phenylsulfonyl)-, (4E) - (9CI) (CA INDEX NAME)

613674-38-7P 613674-40-1P 613674-42-3P 613674-44-5P 613674-46-7P 651310-61-1P 651310-62-2P 651310-63-3P 651310-64-4P 651310-65-5P 651310-66-6P 651310-67-7P 651310-68-8P 651310-69-9P 651310-70-2P 651310-71-3P 651310-72-4P 651310-73-5P 651310-74-6P 651310-75-7P 651310-76-8P 651310-77-9P 651310-78-0P 651310-79-1P 651310-80-4P 651310-81-5P 651310-82-6P

RN 613674-40-1 CAPLUS
CN 4H-Pyrido[1,2-a]pyrimidin-4-imine, 8-ethyl-2-(methylthio)-3(phenylsulfonyl)- (9CI) (CA INDEX NAME)

(phenylsulfonyl) - (9CI) (CA INDEX NAME)

RN 613674-42-3 CAPLUS
CN 4H-Pyrido[1,2-a]pyrimidin-4-imine, 9-bromo-7-methyl-2-(methylthio)-3(phenylsulfonyl)- (9CI) (CA INDEX NAME)

RN 613674-44-5 CAPLUS CN 4H-Pyrimido[2,1-a]isoquinolin-4-imine, 2-(methylthio)-3-(phenylsulfonyl)-(9CI) (CA INDEX NAME)

RN 613674-46-7 CAPLUS

CN 4H-Pyrido[1,2-a]pyrimidin-4-imine, 2-(methylthio)-3-(2-naphthalenylsulfonyl)- (9CI) (CA INDEX NAME)

O NH NH NO Mes N

RN 651310-61-1 CAPLUS

CN . INDEX NAME NOT YET ASSIGNED

NH SMe O CI

RN 651310-62-2 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

RN 651310-63-3 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

RN 651310-64-4 CAPLUS CN INDEX NAME NOT YET ASSIGNED

N SMe O C1
N SMe O C1
N NH

RN 651310-65-5 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 651310-66-6 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 651310-67-7 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 651310-68-8 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

RN 651310-69-9 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{Me} & \text{SMe} \\ \hline & \text{O} \\ \text{N} & \text{S-Ph} \\ \hline & \text{NH} & \text{O} \\ \end{array}$$

RN 651310-70-2 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

RN 651310-71-3 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

RN 651310-72-4 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

RN 651310-73-5 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

RN 651310-74-6 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} n-\text{Pr} & \text{SMe} \\ \hline & \text{O} \\ & \text{N} & \text{S-Ph} \\ \\ & \text{NH} & \text{O} \\ \end{array}$$

RN 651310-75-7 CAPLUS

CN 4H-Pyrido[1,2-a]pyrimidine-7-carboxylic acid, 4-imino-2-(methylthio)-3-(phenylsulfonyl)-, methyl ester (9CI) (CA INDEX NAME)

RN 651310-76-8 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} Me & SMe \\ \hline N & SMe \\ \hline N & S-Ph \\ \hline NH & O \\ \end{array}$$

RN 651310-77-9 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{Ph-CH}_2\text{-O} \\ \hline \\ N \\ N \\ NH \\ O \\ \end{array} \begin{array}{c|c} \text{SMe} \\ O \\ S \\ -\text{Ph} \\ O \\ \end{array}$$

RN 651310-78-0 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 651310-77-9

CMF C22 H19 N3 O3 S2

$$\begin{array}{c|c} \text{Ph-CH}_2\text{-O} & & \text{SMe} \\ \hline & N & & \text{O} \\ & N & & \parallel \\ & N & & \parallel \\ & N & & \text{O} \end{array}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 651310-79-1 CAPLUS

CN 4H-Pyrimido[2,1-a]isoquinolin-4-imine, 2-(methylthio)-3-(phenylsulfonyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 613674-44-5 CMF C19 H15 N3 O2 S2

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 651310-80-4 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

RN 651310-81-5 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 651310-80-4

CMF C18 H14 N4 O2 S2

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 651310-82-6 CAPLUS

CN 4H-Pyrido[1,2-a]pyrimidine-7-carboxamide, 4-imino-2-(methylthio)-3-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

RN 651310-83-7 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 651310-82-6

CMF C16 H14 N4 O3 S2

$$\begin{array}{c|c} & & & & \\ & & & \\ H_2N-C & & & & \\ \parallel & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 651310-84-8 CAPLUS

CN 4H-Pyrido[1,2-a]pyrimidin-2-amine, 4-imino-N-methyl-3-(phenylsulfonyl)-(9CI) (CA INDEX NAME)

RN 651310-85-9 CAPLUS

CN 4H-Pyrido[1,2-a]pyrimidin-2-amine, N-ethyl-4-imino-3-(phenylsulfonyl)-(9CI) (CA INDEX NAME)

RN 651310-87-1 CAPLUS

CN 4H-Pyrido[1,2-a]pyrimidin-2-amine, 4-imino-7-methyl-N-(5-methyl-2-pyridinyl)-3-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

RN 651310-88-2 CAPLUS

CN 4H-Pyrido[1,2-a]pyrimidin-2-amine, 4-imino-7-methyl-N-(5-methyl-2-pyridinyl)-3-(phenylsulfonyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 651310-87-1 CMF C21 H19 N5 O2 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 651310-89-3 CAPLUS
CN Ethanol, 2-[[4-imino-3-(phenylsulfonyl)-4H-pyrido[1,2-a]pyrimidin-2-yl]amino]- (9CI) (CA INDEX NAME)

RN 651310-91-7 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 651310-93-9 CAPLUS CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 651310-92-8

CMF C16 H15 N3 O3 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 651310-94-0 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

RN 651310-95-1 CAPLUS

CN Methanamine, N-[2-(methylthio)-3-(phenylsulfonyl)-4H-pyrido[1,2-a]pyrimidin-4-ylidene]- (9CI) (CA INDEX NAME)

RN 651310-96-2 CAPLUS

CN Acetamide, N-[2-(methylthio)-3-(phenylsulfonyl)-4H-pyrido[1,2-a]pyrimidin-4-ylidene]- (9CI) (CA INDEX NAME)

RN 651310-97-3 CAPLUS

CN 4H-Pyrido[1,2-a]pyrimidin-4-one, 2-(methylthio)-3-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

RN 651310-98-4 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 651310-69-9 CMF C16 H15 N3 O2 S2

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 651310-99-5 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 651310-70-2 CMF C15 H12 Br N3 O2 S2

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 651311-00-1 CAPLUS CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 651310-71-3 CMF C15 H12 C1 N3 O2 S2

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 651311-01-2 CAPLUS

## CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 651310-72-4 CMF C16 H15 N3 O2 S2

CM 2

CRN 76-05-1 CMF C2 H F3 O2

## 10/620,240

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2003:797156 CAPLUS

DN 139:323484

TI Identification of a Potent and Selective 5-HT6 Antagonist: One-Step Synthesis of (E)-3-(Benzenesulfonyl)-2-(methylsulfanyl)pyrido[1,2-a]pyrimidin-4-ylidenamine from 2-(Benzenesulfonyl)-3,3-bis(methylsulfanyl)acrylonitrile

AU Wu, Yong-Jin; He, Huan; Hu, Shuanghua; Huang, Yazhong; Scola, Paul M.; Grant-Young, Katharine; Bertekap, Robert L.; Wu, Dedong; Gao, Qi; Li, Yi; Klakouski, Cheryl; Westphal, Ryan S.

CS Bristol-Myers Squibb Pharmaceutical Research Institute, Wallingford, CT, 06492, USA

SO Journal of Medicinal Chemistry (2003), 46(23), 4834-4837 CODEN: JMCMAR; ISSN: 0022-2623

PB American Chemical Society

DT Journal

LA English

AB A series of 2-(methylsulfenyl)pyrido[1,2-a]pyrimidin-4-ylidenamines, e.g. I (R1 = n-Pr, Ph, 2-naphthyl; R2 = H, F, Me; R3 = H, Et; R4 = H, Br), was synthesized and I [R1 = Ph, R2 = R3 = R4 = H; (II)] was found to be a potent and selective 5-HT6 antagonist. A one-step synthesis of II is described.

IT 613674-38-7P 613674-40-1P 613674-42-3P 613674-44-5P 613674-46-7P 614732-18-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. of sulfonyl-substituted (imino) (methylsulfenyl)pyridopyrimidine s as selective 5-HT6 antagonists)

RN 613674-38-7 CAPLUS

CN 4H-Pyrido[1,2-a]pyrimidin-4-imine, 7-fluoro-2-(methylthio)-3-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

RN 613674-40-1 CAPLUS

CN 4H-Pyrido[1,2-a]pyrimidin-4-imine, 8-ethyl-2-(methylthio)-3-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

RN 613674-42-3 CAPLUS

CN 4H-Pyrido[1,2-a]pyrimidin-4-imine, 9-bromo-7-methyl-2-(methylthio)-3-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

RN 613674-44-5 CAPLUS

CN 4H-Pyrimido[2,1-a]isoquinolin-4-imine, 2-(methylthio)-3-(phenylsulfonyl)(9CI) (CA INDEX NAME)

RN 613674-46-7 CAPLUS

CN 4H-Pyrido[1,2-a]pyrimidin-4-imine, 2-(methylthio)-3-(2-naphthalenylsulfonyl)- (9CI) (CA INDEX NAME)

RN 614732-18-2 CAPLUS

CN 4H-Pyrido[1,2-a]pyrimidin-4-imine, 2-(methylthio)-3-(phenylsulfonyl)-, (4E)- (9CI) (CA INDEX NAME)

RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L1 STRUCTURE UPLOADED

L2 2 S L1 SSS SAM

L3 . 45 S L1 SSS FUL

FILE 'CAPLUS' ENTERED AT 16:17:40 ON 26 FEB 2004

L4 2 S L3

FILE 'CAOLD' ENTERED AT 16:18:13 ON 26 FEB 2004

=> s 13

L5 0 L3

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